Large magnetoresistance in bcc Co/MgO/Co and FeCo/MgO/FeCo tunneling junctions *

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Abstract

By use of first-principles electronic structure calculations, we predict that the magnetoresistance of the bcc Co(100)/MgO(100)/bcc Co(100) and FeCo(100)/MgO(100)/FeCo(100) tunneling junctions can be several times larger than the very large magnetoresistance predicted for the Fe(100)/MgO(100)/Fe(100) system. The origin of this large magnetoresistance can be understood using simple physical arguments by considering the electrons at the Fermi energy travelling perpendicular to the interfaces. For the minority spins there is no state with Δ_1 symmetry whereas for the majority spins there is only a Δ_1 state. The Δ_1 state decays much more slowly than the other states within the MgO barrier. In the absence of scattering which breaks the conservation of momentum parallel to the interfaces, the electrons travelling perpendicular to the interfaces undergo total reflection if the moments of the electrodes are anti-parallel. These arguments apply equally well to systems with other well ordered tunnel barriers and for which the most slowly decaying complex energy band in the barrier has Δ_1 symmetry. Examples include systems with (100) layers constructed from Fe, bcc Co, or bcc FeCo electrodes and Ge, GaAs, or ZnSe barriers.

Spin dependent tunneling junctions formed by trilayers of FM/insulator/FM or FM/semiconductor/FM where FM represents a ferromagnet have been shown to have relatively large magnetoresistance[1,2,3,4]. Much larger magnetoresistances have been predicted in recent calculations on epitaxial spin tunneling systems[5,6,7,8,9]. We have earlier[6] calculated the electronic structure and the spin-dependent tunneling conductance of Fe(100)/MgO(100)/Fe(100) sandwiches, using the first-principles layer-KKR[5] approach. It was found that for this system, the majority spin conductance when the two Fe layers are aligned is dominated by contributions from $k_{\|} = 0$, *i.e.* by electrons travelling perpendicular to the interface. The importance of the complex energy bands within the barrier in determining the rate of decay of electrode Bloch states of similar symmetry[6,9] was also emphasized. This effect of wave function symetry was explained in terms of symmetry induced oscillations of the wave function in the plane of the interface[10]. In addition, these calculations predicted a number of surprising phenomena such as quantum interference between tunneling states. Recently, calculations performed independently by Mathon and Umerski[8] have also predicted very large TMR for the Fe(100)/MgO(100)/Fe(100) system.

These earlier works predicted TMR ratios as high as 6000%(defined as the ratio of the change in resistance to the parallel resistance). These are much larger than the ratios that have been been reported[11,12,13] to date which are approximately 100% or less. It is believed that at least part of the reason for the observed TMR being lower than that calculated is a strong affinity between Fe and O which causes a partial layer of FeO to form at the interface between Fe and MgO[14,15]. Recently, we have performed calculations which showed that an FeO layer would indeed, dramatically lower the TMR[7].

In this paper we consider the symmetric junctions bcc Co(100)/MgO(100)/Co(100) and FeCo(100)/MgO(100)/FeCo(100) with epitaxial lattices. In the latter system, the electrodes are formed by an ordered FeCo bcc alloy. Effects of disorder are not included in the present calculations. It is possible that Co(100)/MgO(100) or FeCo(100)/MgO(100) may be easier to grow without an interfacial transition metal oxide layer than Fe(100)/MgO(100). Indeed, preliminary reports of large TMR in systems of the form FeCo(100)/MgO(100)/FeCo(100) and FeCo(100)/MgO(100)/AlGaAs(100) have been presented[16,17]. In these cases, FeCo seems to have been a crystalline bcc alloy with at least some substitutional disorder.

Similarly to our previous calculations[6], the electrode layers of bulk bcc cobalt are fixed at the lattice constant of 2.82 Å, while the lattice constant of bulk bcc FeCo is chosen to be 2.86 Å. The MgO lattice constant is taken to be a factor of $\sqrt{2}$ larger than that of the bulk electrodes,

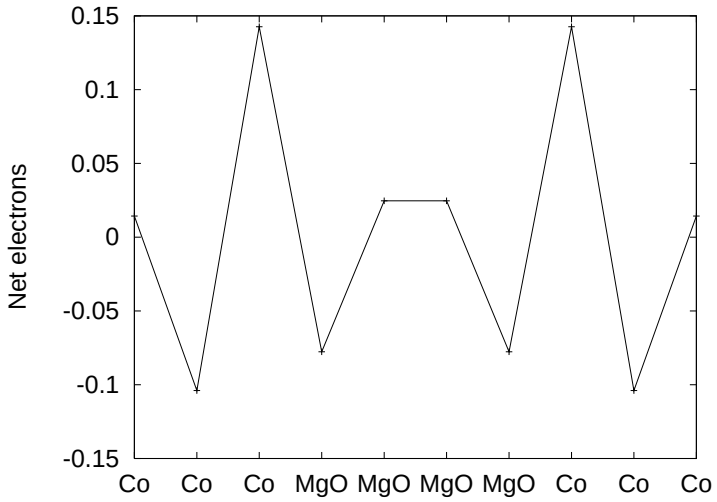

FIG. 1: Net charge on each atomic layer of the Co/MgO/Co tunnel junction.

therefore the (100) layers of the two materials can be matched epitaxially. We assume no vertical relaxations between the layers. In order to fill the space with a minimal amount of overlap between the spheres, an empty sphere is inserted between the MgO and the electrode layers at the MgO/Co or MgO/FeCo interface.

The self-consistent calculation is performed in the same manner as in Refs.[6,7]. We limited our calculations within magnetic configuration space in the sense that all electron spins are assumed collinear. We also assumed that the magnetic order has the same periodicity as the two-dimensional lattice thus disallowing antiferromagnetic ordering within the same atomic layer. Antiferromagnetic coupling between layers is allowed, however. The tunneling conductance is calculated using the same approach as in Ref.[6]. It uses the LKKR code which implements the Landauer-Büttiker conductance formalism[18,19] within the first-principles KKR framework.

We find that the charge rearrangement necessary to correctly offset the bands of the MgO relative to those of Co leads to very little charge transfer between layers (Fig. 1), similar to the result we obtained for the Fe/MgO interface. We also found little charge transfer at the FeCo/MgO interface.

The tunneling conductance for the three types of electrodes, bcc Fe(100), bcc(Co)100 and B2 FeCo(100) all using an 8ml MgO(100) barrier are shown in Table I. Although our physical arguments emphasize $k_{\|} = 0$, it should be emphasized that the results presented in Table I, resulted from an integral over the entire two dimensional Brillouin zone with 8256 k-points in $1/8$th of the zone. For the minority channel, interfacial resonance states generate extremely sharp peaks as a

TABLE I: Tunneling conductivity (in $1/\Omega m^2$) for various spin channels for the Co/MgO/Co and FeCo/MgO/FeCo tunnel junctions. Each junction contains 8 atomic layers of MgO. Resonant state contributions to the minority spin channel have been removed. Results for Fe/MgO/Fe are also listed for comparison. The electrode materials are all assumed to have the bcc phase and all interfaces are normal to the (100) direction.

Spin alignment	up-up	down-down	up-down (down-up)	σ_P/σ_{AP}
FeCo/MgO/FeCo	1.19×10^9	2.55×10^6	1.74×10^6	353.5
Co/MgO/Co	8.62×10^8	7.51×10^7	3.60×10^6	147.2
Fe/MgO/Fe	2.55×10^9	7.08×10^7	2.41×10^7	54.3

function of $\mathbf{k}_\parallel$. The contributions from these peaks have been omitted because they are difficult to calculate accurately. If they had been included, the calculated TMR would have been slightly higher because for the Co and FeCo electrodes they contribute to the minority parallel conductance but do not contribute significantly to the anti-parallel conductance.

The tunneling density of states (TDOS) is defined as the electron density of states at each layer due to a single incident Bloch state from the left Fe (Co or CoFe) lead. On each layer, the TDOS is roughly proportional to the modular square of the wave function that matches to the incident Bloch state. The TMR is dominated by the parallel majority spin conductance, which in turn is dominated by the contribution from $k_\parallel = 0$. As shown in Figs. 2 and 3, the majority spin TDOS for the Δ_1 state decreases much more slowly in the MgO layer than the states with different symmetries. This is true for both the Co/MgO/Co stack and the FeCo/MgO/FeCo stack and is similar to the result we obtained for the Fe/MgO/Fe tunnel junction. A striking feature that distinguishes Co/MgO/Co and FeCo/MgO/FeCo from earlier results for Fe/MgO/Fe, is that for the antiparallel spin alignment, *all* states are completely reflected at $k_\parallel = 0$. This effect is the reason for the much larger conductance ratio for Co/MgO/Co and FeCo/MgO/FeCo than Fe/MgO/Fe tunnel junctions.

The total reflection of the tunneling electrons at $k_\parallel = 0$ for antiparallel spin alignment is due to the fact that there are no Bloch eigenstates in the minority spin channel with Δ_1 symmetry. This results from the hybridization of the "s-band" with the d-bands. In a generic bcc transition metal electronic structure the s-band typically starts from the Γ point a few eV below the d-bands. Its energy rises rapidly with k until it encounters the d-bands at which point it flattens out and ends at the Brillouin zone boundary near the bottom of the d-band complex. Starting above the d-band

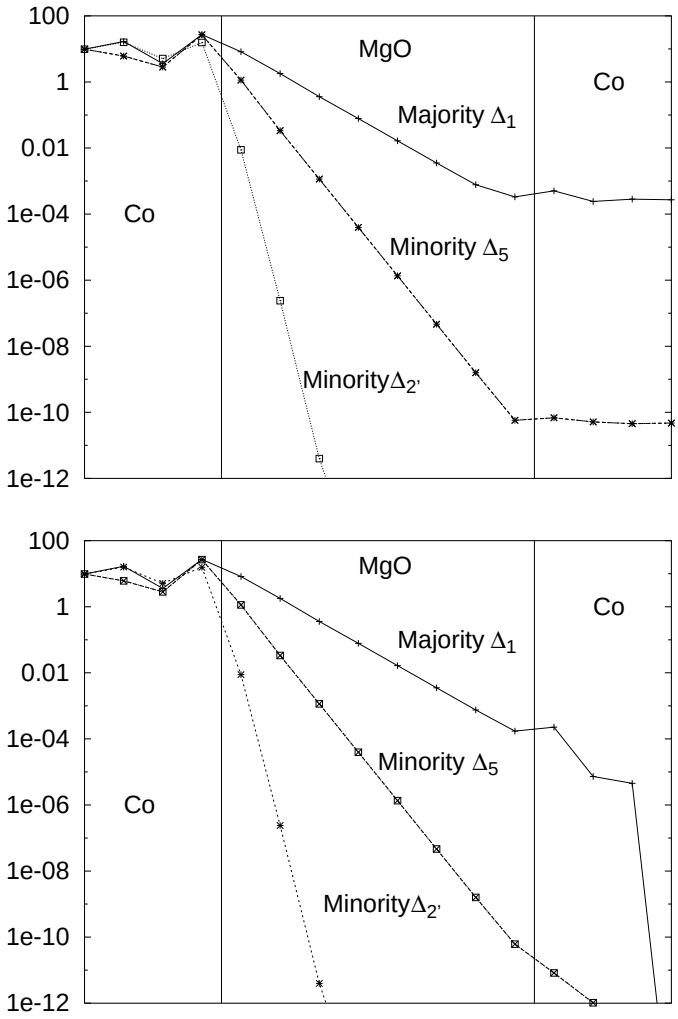

FIG. 2: Tunneling density of states on each atomic layer at $k_{||} = 0$ for Co/MgO/Co tunnel junction. Top panel, parallel spin alignment, bottom panel, antiparallel spin alignment

complex, the "s-band" can also be followed downward in energy. It is again highly dispersive until it approaches the d-band complex at which point it flattens out and intersects the zone center at the $\Gamma_{2'}$ point. In the (100) direction, the "s-band" is the one with Δ_1 symmetry and there is a range of energy over which there is no Δ_1 band. For bcc Co and bcc FeCo, the spin splitting is such that no Δ_1 band crosses the minority electron Fermi energy and the only band that crosses the majority Fermi energy is a Δ_1 band.

A consequence of this is that the minority states at $k_{||} = 0$ have no s component. Only the Δ_1 wave functions are compatible with $\ell = 0$ symmetry when expanded about an atomic center. The absence of s-DOS is evident in the plots of the partial DOS at $k_{||} = 0$ of the minority spin electrons

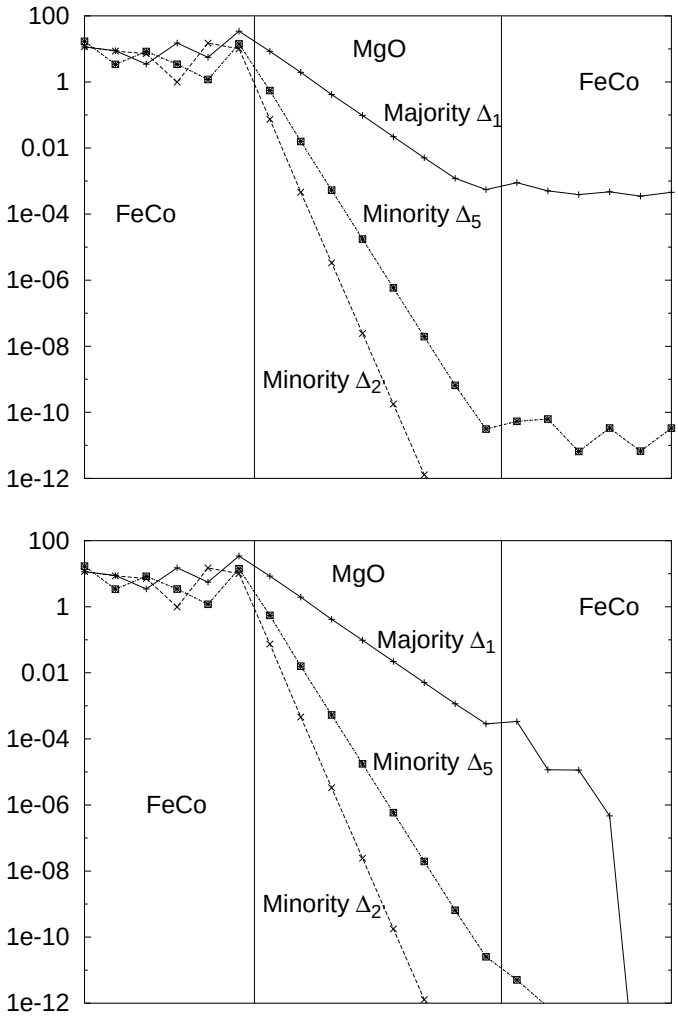

FIG. 3: Tunneling density of states on each atomic layer at $k_{||} = 0$ for FeCo/MgO/FeCo tunnel junction. Top panel, parallel spin alignment, bottom panel, antiparallel spin alignment

in Figs. 4 and 5. In both plots, the Fermi energy (indicated by the vertical bar) falls within the energy gap of the s partial DOS. Because all of the slowly decaying tunneling states within the MgO layer must have s component due to the symmetry of the wave function in MgO, a Bloch state with zero s component decays very rapidly in the MgO layer. Conversely, in the absence of any Bloch states with a nonzero s component, a tunneling state can not exit the MgO layer.

Half-metallic ferromagnetic electrodes, (*i.e.* ferromagnets with states of only one spin channel at the Fermi energy) are not required in order to obtain very large TMR. If one can achieve sufficiently good two dimensional periodicity within the barrier and near the interface that $k_{||}$ is reasonably well conserved, *i.e.* the scattering is mostly specular, then one may take advantage of

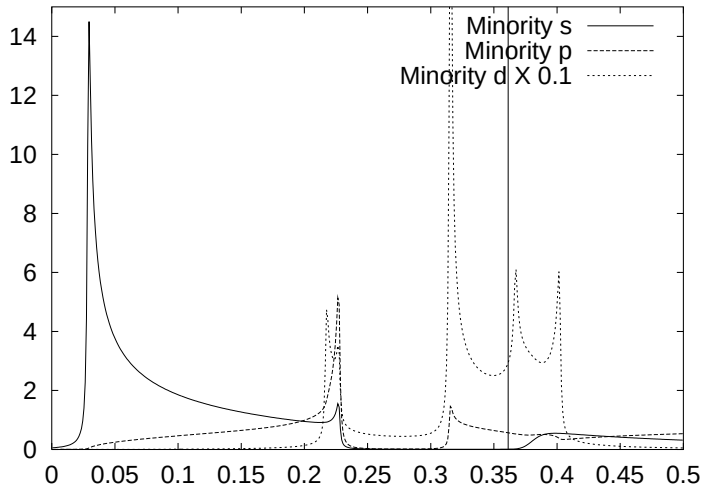

FIG. 4: Partial density of states at $k_{\|} = 0$ in bulk bcc cobalt.

a class of electrode-barrier combinations in which some of the states of one spin channel decay much more slowly in the barrier than those of the other. In addition, a total reflection of the electrons traveling perpendicular to the interface when the moments of the electrodes are antiparallel can further increase the TMR by several fold.

This argument is, of course, more speculative in the presence of disorder. Some types of disorder, however, may not completely eliminate the effect. For strong magnetic alloys, *i.e.* those with filled majority d-bands, the moments are such that the bands match extremely well in the majority channel. Therefore, $k_{\|}$ conservation arguments can be applied to majority electrons. The problem will be in the minority channel where the scattering is expected to be relatively strong. Even there however, the bcc Co and FeCo electrodes should offer the possibility for relatively large TMR. Consider the case of anti-parallel alignment. Majority electrons injected from the left electrode (as in the lower pannels of Figures 2 and 3) will decay slowly in the MgO barrier. When they encounter the right electrode, however, the (initially) Δ_1 states that would decay exponentially if the electrode were well ordered will, we speculate, continue do so for several layers until diffuse scattering converts a significant fraction of the surviving flux into symmetries that can propagate.

Finaly, we note that the total reflection depends on the absence of the Δ_1 band for the minority spin in the cubic (100) direction. The fact that the measurements of FeCo/MgO/FeCo junctions[17] showed greatly reduced TMR for the (110) textured samples and for non-bcc Co rich electrodes confirms that the role of Co is more than simply preventing the formation of an FeO layer, and the total reflection of the $\bar{\Gamma}$ electrons may play a crucial role in achieving the high TMR.

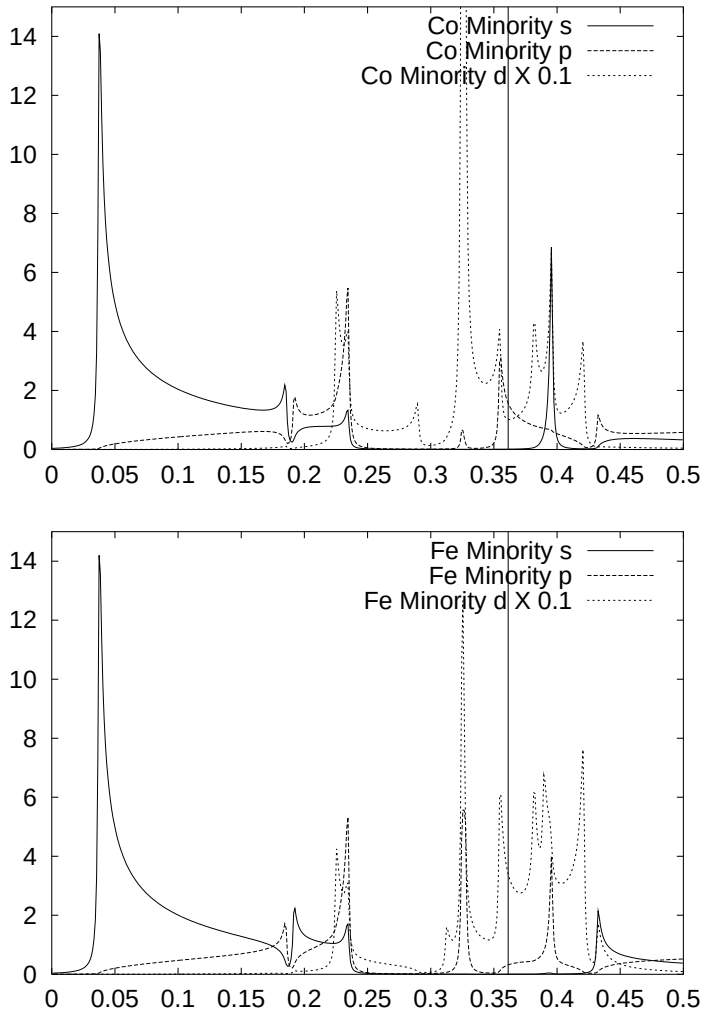

FIG. 5: Partial density of states at $k_{\|} = 0$ in bulk bcc FeCo. Top panel, Co sublattice, bottom panel, Fe sublattice

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